

L Number	Hits	Search Text	DB	Time stamp
1	110	acorus near2 calamus	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/08/19 17:35
3	21	(acorus near2 calamus) and \$4asarone	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/08/19 17:32
4	89	(acorus near2 calamus) not \$4asarone	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/08/19 17:36
5	149	sweet near2 flag	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/08/19 17:36
6	406282	hydrogenat\$6 or h2!	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/08/19 17:37
7	13	((acorus near2 calamus) or (sweet near2 flag)) same (hydrogenat\$6 or h2!)	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/08/19 17:37
2	38	\$4asarone	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/08/19 17:38

09/652,376

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PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

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NEWS	2	"Ask CAS" for self-help around the clock
NEWS	3 May 12	EXTEND option available in structure searching
NEWS	4 May 12	Polymer links for the POLYLINK command completed in REGISTRY
NEWS	5 May 27	New UPM (Update Code Maximum) field for more efficient patent SDIs in CAPlus
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NEWS	9 Jul 12	BEILSTEIN enhanced with new display and select options, resulting in a closer connection to BABS
NEWS	10 Jul 30	BEILSTEIN on STN workshop to be held August 24 in conjunction with the 228th ACS National Meeting
NEWS	11 AUG 02	IFIPAT/IFIUDB/IFICDB reloaded with new search and display fields
NEWS	12 AUG 02	CAPlus and CA patent records enhanced with European and Japan Patent Office Classifications
NEWS	13 AUG 02	STN User Update to be held August 22 in conjunction with the 228th ACS National Meeting
NEWS	14 AUG 02	The Analysis Edition of STN Express with Discover! (Version 7.01 for Windows) now available
NEWS	15 AUG 04	Pricing for the Save Answers for SciFinder Wizard within STN Express with Discover! will change September 1, 2004
NEWS EXPRESS	JULY 30	CURRENT WINDOWS VERSION IS V7.01, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 17:48:27 ON 19 AUG 2004

09/652,376

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 17:48:38 ON 19 AUG 2004

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 18 AUG 2004 HIGHEST RN 728239-10-9

DICTIONARY FILE UPDATES: 18 AUG 2004 HIGHEST RN 728239-10-9

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>Testing the current file.... screen

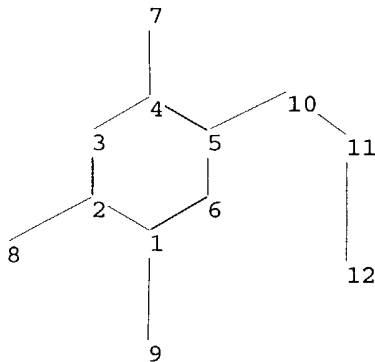
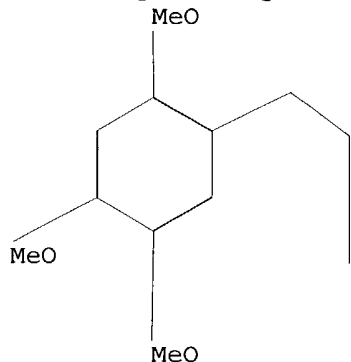
ENTER SCREEN EXPRESSION OR (END):end

=> screen 1992 OR 2016 OR 2021 OR 2026 OR 1839

L1 SCREEN CREATED

=>

Uploading C:\Program Files\Stnexp\Queries\09652376.str



chain nodes :

7 8 9 10 11 12

ring nodes :

1 2 3 4 5 6

chain bonds :

1-9 2-8 4-7 5-10 10-11 11-12

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

09/652,376

exact bonds :

1-9 2-8 4-7 5-10 10-11 11-12

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS

L2 STRUCTURE UPLOADED

=> que L2 NOT L1

L3 QUE L2 NOT L1

=> s l3

SAMPLE SEARCH INITIATED 17:48:58 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 58 TO ITERATE

100.0% PROCESSED 58 ITERATIONS

8 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 704 TO 1616

PROJECTED ANSWERS: 8 TO 329

L4 8 SEA SSS SAM L2 NOT L1

=> s l3 ful

FULL SEARCH INITIATED 17:49:03 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1215 TO ITERATE

100.0% PROCESSED 1215 ITERATIONS

175 ANSWERS

SEARCH TIME: 00.00.01

L5 175 SEA SSS FUL L2 NOT L1

=> d scan

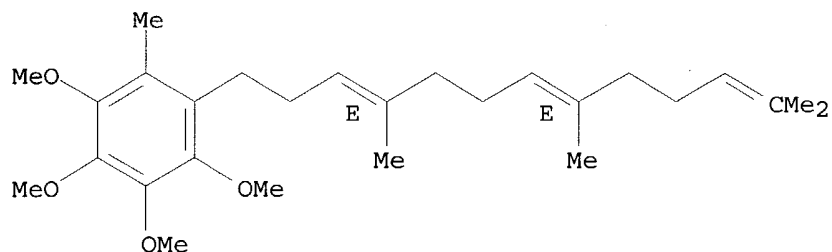
L5 175 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN Benzene, 1,2,3,4-tetramethoxy-5-methyl-6-[(3E,7E)-4,8,12-trimethyl-3,7,11-tridecatrienyl]- (9CI)

MF C27 H42 O4

Double bond geometry as shown.

09/652,376



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> s l3 ful css

FULL SEARCH INITIATED 17:49:30 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1215 TO ITERATE

100.0% PROCESSED 1215 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

L6 1 SEA CSS FUL L2 NOT L1

=> d

L6 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 6906-65-6 REGISTRY

CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

OTHER NAMES:

CN 1,2,4-Trimethoxy-5-propylbenzene

CN 1-(2,4,5-Trimethoxyphenyl)propane

CN Dihydroasarone

FS 3D CONCORD

MF C12 H18 O3

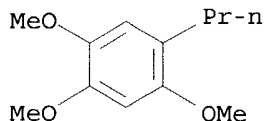
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, TOXCENTER, USPAT2, USPATFULL

(*File contains numerically searchable property data)

DT.CA CAplus document type: Journal; Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

RL.NP Roles from non-patents: BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PRP (Properties); RACT (Reactant or reagent); NORL (No role in record)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

13 REFERENCES IN FILE CA (1907 TO DATE)

13 REFERENCES IN FILE CAPLUS (1907 TO DATE)

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

09/652,376

=> file caplus caold

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

312.61

312.82

FILE 'CAPLUS' ENTERED AT 17:50:03 ON 19 AUG 2004

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FILE 'CAOLD' ENTERED AT 17:50:03 ON 19 AUG 2004

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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=> s 6906-65-6

L7 14 6906-65-6

=> dup rem l7

DUPLICATE IS NOT AVAILABLE IN 'CAOLD'.

ANSWERS FROM THESE FILES WILL BE CONSIDERED UNIQUE

PROCESSING COMPLETED FOR L7

L8 14 DUP REM L7 (0 DUPLICATES REMOVED)

=> d 1-14 bib ab fhitrstr

L8 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2003:777737 CAPLUS

DN 139:292100

TI Formation of neolignan by DDQ mediated dimerization of dihydroasarone

IN Sinha, Arun Kumar; Joshi, Bhupendra Prasad; Acharya, Ruchi

PA Council of Scientific and Industrial Research, India

SO PCT Int. Appl., 37 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

PATENT NO.

KIND

DATE

APPLICATION NO.

DATE

PI	WO 2003080551	A1	20031002	WO 2002-IN73	20020327
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

PRAI WO 2002-IN73

20020327

OS CASREACT 139:292100

AB The present invention relates to a novel neolignan 3-ethyl-2-methyl-3-(2'',4'',5''-trimethoxyphenyl)-1-(2',4',5'-trimethoxyphenyl)-1-propene and a process for the preparation of high purity, high yield neolignan, α -asarone, and 2,4,5-trimethoxyphenylpropionone from β -asarone or β -asarone rich Acorus calamus oil containing α - and γ -asarone by hydrogenating and dimerizing by treatment with DDQ in presence of an organic acid.

IT 6906-65-6P

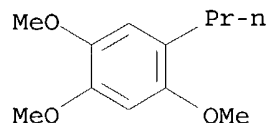
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic

09/652,376

preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of neolignan by DDQ mediated dimerization of dihydroasarone)

RN 6906-65-6 CAPLUS

CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2003:777446 CAPLUS

DN 139:292099

TI DDQ-mediated one step dimerization of β -asarone or β -asarone rich Acorus calamus oil in the formation of novel neolignan

IN Sinha, Arun Kumar; Joshi, Bhupendra Prasad; Acharya, Ruchi

PA Council of Scientific & Industrial Research, India

SO U.S. Pat. Appl. Publ., 20 pp.

CODEN: USXXCO

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2003187306	A1	20031002	US 2002-108269	20020328
	US 2004049085	A1	20040311	US 2003-660556	20030912
PRAI	US 2002-108269	B3	20020328		

OS CASREACT 139:292099

AB The present invention relates to a novel neolignan, 3-ethyl-2-methyl-3-(2'',4'',5''-trimethoxyphenyl)-1-(2',4',5'-trimethoxyphenyl)-1-(2',4',5'-trimethoxy)phenyl-1-propene [NEOLASA-I (I)], and a process for the preparation of high purity, higher yield neolignan, α -asarone, 2,4,5-trimethoxy-phenylpropionone from β -asarone (II) or β -asarone rich Acorus calamus oil containing α - and γ -asarone by hydrogenating and dimerizing by treatment with DDQ in presence of an organic acid.

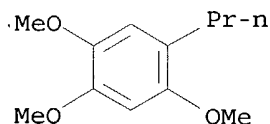
IT 6906-65-6P, Dihydroasarone

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and dimerization of, with DDQ; DDQ-mediated one step dimerization of β -asarone or β -asarone rich Acorus calamus oil in the formation of novel neolignans)

RN 6906-65-6 CAPLUS

CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



L8 ANSWER 3 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2003:524051 CAPLUS

DN 139:90404

TI Process for the preparation of pharmacologically active α -asarone

09/652,376

from toxic β -asarone-rich Acorus calamus oil
IN Sinha, Arun Kumar; Joshi, Bhupendra Prasad; Acharya, Ruchi
PA Council of Scientific & Industrial Research, India
SO U.S., 22 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6590127	B1	20030708	US 2002-107844	20020328
	WO 2003082786	A1	20031009	WO 2002-IN94	20020328
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRAI US 2002-107844 A 20020328

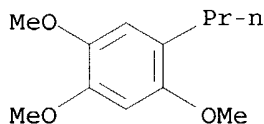
AB The present invention relates to a process for the preparation of high purity and yield α -asarone, trans-2,4,5-trimethoxycinnamaldehyde, and 2,4,5-trimethoxyphenylpropanone, from β -asarone or β -asarone-rich Acorus calamus oil containing α and γ -asarone by hydrogenation, followed by treatment with a dehydrogenating agent dichlorodicyanobenzoquinone (DDQ) with or without solid support of silica gel or alumina in dry organic solvent. α -Asarone can also be obtained by treating the hydrogenated product of β -asarone or β -asarone-rich A. calamus oil with DDQ in an aqueous organic solvent to obtain an intermediate 2,4,5-trimethoxyphenylpropanone, which in turn is reduced with sodium borohydride to obtain the corresponding 2,4,5-trimethoxyphenylpropanol and followed by final treatment with a dehydrating agent.

IT 6906-65-6P, Dihydroasarone

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pharmacol. active α -asarone by hydrogenation of toxic β -asarone-rich Acorus calamus oil)

RN 6906-65-6 CAPLUS

CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



RE.CNT 91 THERE ARE 91 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:717107 CAPLUS

DN 137:234008

TI Production of substituted trans-cinnamaldehydes and yellow dyes from phenylpropane derivatives

IN Sinha, Arun Kumar; Joshi, Bhupendra Prasad; Dogra, Ruchi

PA India

SO U.S. Pat. Appl. Publ., 15 pp.

09/652,376

CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2002133045	A1	20020919	US 2001-805832	20010314
	US 6566557	B2	20030520		
	GB 2373252	A1	20020918	GB 2001-6430	20010315
	DE 10113506	A1	20020926	DE 2001-10113506	20010320
	BR 2001003269	A	20021203	BR 2001-3269	20010322
	FR 2822473	A1	20020927	FR 2001-3984	20010323
	WO 2002072709	A1	20020919	WO 2001-IN104	20010521

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRAI US 2001-805832 A 20010314

OS CASREACT 137:234008; MARPAT 137:234008

AB The invention relates to the production of substituted trans-cinnamaldehydes (I, R1 = trans-CH:CHCHO; R2, R3, R4, R5, R6 = H, alkyl, alkoxy, or adjacent groups may form methylenedioxy) by oxidizing the corresponding phenylpropane derivs. using an oxidizing agent such as 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ), p-chloranil, pyridinium chlorochromate, tert-BuOOH, or CrO3 with a catalytic amount of inorg./organic acid (optionally on alumina, celite, and silica gel as a solid support for microwave irradiation); the trans-cinnamaldehydes and natural yellow dyes are obtained in high yield ranging from 68-82%. In an example, yellow 2,4,5-trimethoxycinnamaldehyde was obtained in 84% yield by oxidation of 1-(2,4,5-trimethoxyphenyl)propane in the presence of DDQ and acetic acid.

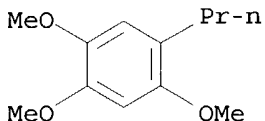
IT 6906-65-6, 1-(2,4,5-Trimethoxyphenyl)propane

RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; in production of cinnamaldehydes and yellow dyes by oxidation of phenylpropane derivs.)

RN 6906-65-6 CAPLUS

CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



L8 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:221245 CAPLUS

DN 136:247399

TI Process for the preparation of 1-propyl-2,4,5-trimethoxybenzene from toxic β -asarone of Acorus calamus or from crude calamus oil containing β -asarone

IN Sinha, Arun Kumar

PA Council of Scientific and Industrial Research, India

SO U.S. Pat. Appl. Publ., 16 pp., Division of U.S. Ser. No. 652,376.

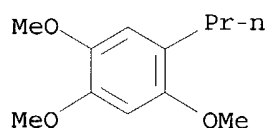
CODEN: USXXCO

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2002035299	A1	20020321	US 2001-957867	20010921
	US 6528041	B2	20030304		
	CN 1340494	A	20020320	CN 2001-119219	20010327
	JP 2002088004	A2	20020327	JP 2001-101894	20010330
	US 2003113275	A1	20030619	US 2003-338327	20030108
PRAI	US 2000-652376	A3	20000831		
	US 2001-957867	A3	20010921		
OS	CASREACT 136:247399				
AB	The invention relates to a process for the preparation of 1-Propyl-2,4,5-trimethoxybenzene useful as a aroma mol. and as a starting material and intermediate for preparation of various drugs. The process comprises providing crude calamus oil or β -asarone in a solvent; hydrogenating the solution in the presence of a catalyst; filtering the catalyst and removing the solvent under reduced pressure; subjecting the reduced calamus oil to column of silica gel chromatog. using an eluent to obtain the desired product in liquid form with 85-97% purity.				
IT	6906-65-6P, Benzene, 1,2,4-trimethoxy-5-propyl- RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of 1-propyl-2,4,5-trimethoxybenzene from toxic β -asarone of Acorus calamus or from crude calamus oil containing β -asarone)				
RN	6906-65-6 CAPLUS				
CN	Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)				



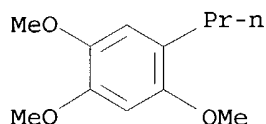
L8 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 2002:710993 CAPLUS
 DN 137:249076
 TI Process for preparation of substituted trans-cinnamaldehyde, a natural yellow dye, from phenylpropane derivatives
 IN Sinha, Arun Kumar; Joshi, Virendara Prasad; Dogura, Ruci
 PA Council of Scientific & Industrial Research, India
 SO Jpn. Kokai Tokkyo Koho, 45 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese

FAN.CNT 1

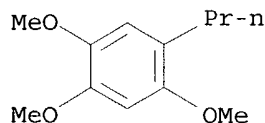
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2002265407	A2	20020918	JP 2001-68716	20010312
PRAI	JP 2001-68716		20010312		
OS	CASREACT 137:249076; MARPAT 137:249076				
AB	A simple and economical process to convert phenylpropane derivs. into corresponding cinnamaldehyde derivs. comprises oxidizing substituted phenylpropane derivs. in presence of a solvent and a catalyst using an oxidizing agent in a mole ratio of 1:1 to 1:8 to the phenylpropane derivs. at a temperature between -15° to 210° for a period of 30 min to 48 h, removing the solvent under reduced pressure and isolating the product to obtain 68-82% of trans-cinnamaldehydes. Thus, a flask containing a mixture of 4-methoxyphenylpropane 2, silica gel 0.5-0.8, 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) 7.5 g and 5-8 mL dioxane was placed inside a microwave oven operating at medium power (600 W) and irradiated for 2-8				

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min to give 68% 4-methoxycinnamaldehyde.
IT 6906-65-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(simple and economical process for preparation of substituted
trans-cinnamaldehyde natural yellow dye from phenylpropane derivs.)
RN 6906-65-6 CAPLUS
CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



L8 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:830461 CAPLUS
DN 136:128585
TI High hypolipidemic activity of saturated side-chain α -asarone
analogues
AU Cruz, Adriana; Garduno, Leticia; Salazar, Maria; Martinez, Elizdath; Diaz,
Francisco; Chamorro, German; Tamariz, Joaquin
CS Departamento de Quimica Organica, Escuela Nacional de Ciencias Biologicas,
IPN. Prol. Carpio y Plan de Ayala, Mexico, 11340, Mex.
SO Medicinal Chemistry Research (2001), 10(9), 587-595
CODEN: MCREEB; ISSN: 1054-2523
PB Birkhaeuser Boston
DT Journal
LA English
AB With the aim of evaluating the pharmacophore potential of the side chain
of α -asarone regarding its high hypolipidemic activity,
 α -asarone analogs (I) were evaluated pharmacol. For I, with a
variable-size side chain, significant decreases in serum cholesterol,
LDL-cholesterol, and triglyceride levels and significant increases in
HDL-cholesterol levels were observed in mice. I were even more active than
 α -asarone in reducing cholesterol. The results suggested that the
length and saturated character of the side chain seem to be a key feature in
improving hypolipidemic activity of I.
IT 6906-65-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
(Biological study); PREP (Preparation)
(high hypolipidemic activity of saturated side-chain α -asarone
analogues)
RN 6906-65-6 CAPLUS
CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

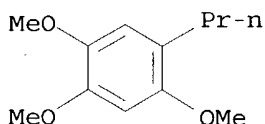


RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:740149 CAPLUS
DN 123:187711
TI Studies on crude drugs effective on visural larva migrans. XVI. Mobility
inhibition and nematocidal activity of asarone and related

09/652,376

phenylpropanoids on second-stage larvae of *Toxocara canis*
AU Sugimoto, Naoki; Goto, Yoshihisa; Akao, Nobuaki; Kiuchi, Fumiyuki; Kondo, Kaoru; Tsuda, Yoshisuke
CS Sch. Med., Kanazawa Univ., Kanazawa, 920, Japan
SO Biological & Pharmaceutical Bulletin (1995), 18(4), 605-9
CODEN: BPBLEO; ISSN: 0918-6158
PB Pharmaceutical Society of Japan
DT Journal
LA English
AB The in vitro effect of asarone, the nematocidal principle of the rhizome of *Acorus calamus*, on second-stage larvae of *Toxocara canis* is composed of two independent actions: one is a fast acting inhibition of the larval mobility and the other is a slow acting larvicidal action. Mobility of the larvae was rapidly inhibited when they were incubated with asarone. Dye exclusion assay revealed that larvae were alive at this stage, and their mobility was restored after the first inhibition, suggesting that this effect was temporary and reversible. However, when the mobility decreased again during prolonged incubation, the cellular viability of larvae disappeared, showing that they were killed by the compound. The above two-stage effect of asarone was almost identical in two geometrical isomers ((E)- and (Z)-asarone). Di- and tri-methoxypropenyl or propylbenzenes carrying two methoxy groups at a vicinal position on a benzene ring showed, more or less, a two-stage effect of this type. These two actions were suggested to be separable by an appropriate modification of the structure.
IT 6906-65-6
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(studies on crude drugs effective on visceral larva migrans. XVI.
Mobility inhibition and nematocidal activity of asarone and related phenylpropanoids on second-stage larvae of *Toxocara canis*)
RN 6906-65-6 CAPLUS
CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

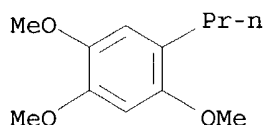


L8 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:138847 CAPLUS
DN 112:138847
TI Potential antipsychotic agents. 5. Synthesis and antidopaminergic properties of substituted 5,6-dimethoxysalicylamides and related compounds
AU Hoegberg, Thomas; Bengtsson, Stefan; De Paulis, Tomas; Johansson, Lars; Stroem, Peter; Hall, Haakan; Oegren, Sven Ove
CS CNS Res. Dev., Astra Res. Cent. AB, Soedertaelje, S-151 85, Swed.
SO Journal of Medicinal Chemistry (1990), 33(4), 1155-63
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
OS CASREACT 112:138847
AB A series of 3-substituted 5,6-dimethoxysalicylamides (I) have been synthesized from the corresponding 2,5,6-trimethoxybenzoic acids. Relaxation times T1 and carbon chemical shifts of the methoxy groups in I showed that the 6-methoxy group adopts a nearly perpendicular orientation and the 5-methoxy group takes on a more coplanar orientation with respect to the ring plane in solution. The salicylamides I display a very high and stereoselective affinity for the [3H]spiperone and [3H]raclopride binding

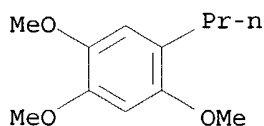
09/652,376

sites in vitro. Regioisomers of salicylamides I also exhibit pronounced, but lower than I, affinity for the [3H]spiperone binding site. The structural requirements were further assessed by studies of the related amino analogs and hydroxy analog. 3-Bromo compound II (FLB 463) was studied in various in vivo models and compared with the dopamine-D2 antagonists sulpiride, raclopride, eticlopride, and haloperidol. The high potency of I to selectively block dopamine-D2 receptors in vitro and in vivo combined with indications on a low potential for motor side effects makes it a very interesting new member of the class of substituted salicylamides.

IT 6906-65-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and carboxylation of)
RN 6906-65-6 CAPLUS
CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



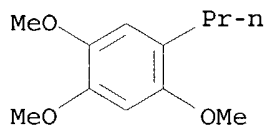
L8 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1983:517832 CAPLUS
DN 99:117832
TI Repellency and toxicity of 55 insect repellents to red-winged blackbirds (*Agelaius phoeniceus*)
AU Schafer, E. W., Jr.; Jacobson, M.
CS Denver Wildl. Res. Cent., USFWS, Denver, CO, 80225, USA
SO Journal of Environmental Science and Health, Part A: Environmental Science and Engineering (1983), A18(4), 493-502
CODEN: JESEDU; ISSN: 0360-1226
DT Journal
LA English
AB A joint research program was initiated in 1979 to investigate the potential avian repellency and toxicity of 55 selected insect repellents originating from or related to naturally occurring chems. Seven of the chems. or exts. tested exhibited avian repellency and 2 of these were considered to be moderately active, with 50% avian repellency concns. of 0.237 (trans-asarone [2883-98-9]) and 0.240% (safrole [94-59-7]). None of the 55 chemical or exts. exhibited acute oral toxicity at ≤ 100 mg/kg to the red-winged blackbird (*Agelaius phoeniceus*).
IT 6906-65-6
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (repellency and toxicity of, to red-winged blackbirds)
RN 6906-65-6 CAPLUS
CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



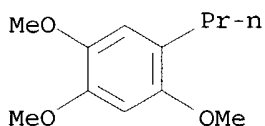
L8 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1982:100901 CAPLUS
DN 96:100901
TI Constituents of *Acorus calamus*: structure of acoramone. Carbon-13 NMR

09/652,376

spectra of cis- and trans-asarone
AU Patra, Amarendra; Mitra, Alok K.
CS Dep. Chem., Univ. Coll. Sci., Calcutta, 700009, India
SO Journal of Natural Products (1981), 44(6), 668-9
CODEN: JNPRDF; ISSN: 0163-3864
DT Journal
LA English
AB The phenylpropane derivs. isoeugenol Me ether, γ -asarone, cis-asarone, trans-asarone, and the new natural product acoramone (I) were isolated along with asarylaldehyde from the oil of *A. calamus*. The ^{13}C -NMR signal assignments of cis- and trans-asarone and their dihydroderivative are also reported.
IT 6906-65-6
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence) (of *Acorus calamus*)
RN 6906-65-6 CAPLUS
CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



L8 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1969:31614 CAPLUS
DN 70:31614
TI Isolation of 2,4,5-trimethoxyallylbenzene from *Caesulia axillaries* oil
AU Devgan, O. N.; Bokadia, M. M.
CS Southern Illinois Univ., Carbondale, IL, USA
SO Australian Journal of Chemistry (1968), 21(12), 3001-3
CODEN: AJCHAS; ISSN: 0004-9425
DT Journal
LA English
AB The phenolic ether obtained from the essential oil of *C. axillaries* has been shown to be 2,4,5-trimethoxyallyl-benzene, on the basis of chemical and spectroscopic evidence. It has tentatively been named as γ -asarone.
IT 6906-65-6P
RL: PREP (Preparation) (from *Caesulia axillaris* oil)
RN 6906-65-6 CAPLUS
CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



L8 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1966:447549 CAPLUS
DN 65:47549
OREF 65:8851d-h
TI Oxa compounds. VI
AU El'tsov, A. V.; Minkin, V. I.; Tsereteli, I. Yu.
CS Oncology Inst., Leningrad
SO Zhurnal Obshchei Khimii (1966), 2(4), 620-7

CODEN: ZOKHA4; ISSN: 0044-460X

DT Journal

LA Russian

AB cf. CA 61, 5640h; 63, 11540d. Heating 10 g. 3,4-(MeO)2C6H3OH with 7.9 g. CH₂:CHCH₂Br and 9 g. powdered K₂CO₃ in Me₂CO 3 hrs. gave 56% 1-allyloxy-3,4-dimethoxybenzene, b₂ 114°, n_{20D} 1.5352, which (6.35 g.) heated with 7 ml. PhNMe₂ 2 hrs. at 200° (bath) gave 95% crude material, which hydrogenated over Pt gave 75% 4,5-dimethoxy-2-propylphenol, m. 76°, and 2% 3,4-dimethoxy-2-propylphenol, m. 94°. The former with Me₂SO₄ in aqueous NaOH 40 min. gave 2,4,5-trimethoxy-1-propylbenzene, b₂ 114°, 1.5190. Heating 18 g. 6-hydroxy-1,4-benzodioxan with 14.5 g. CH₂:CHCH₂Br and 16.3 g. K₂CO₃ in Me₂CO 3 hrs. gave 57% 6-allyloxy-1,4-benzodioxan, b₂ 123°, 1.5505, which heated with PhNMe₂ as above 2 hrs. gave mixed allylphenols, which hydrogenated over Pt gave mixed propylphenols, which methylated with Me₂SO₄ in aqueous NaOH gave unseparable mixture of 6-methoxy-7-propyl-1,4-benzodioxan and the 5-Pr analog, as identified from the N.M.R. spectrum of the mixture; these were formed in approx. equal amts. To 6.3 g. AlCl₃ in PhNO₂ was added with ice cooling 6.6 g. 6-methoxy-1,4-benzodioxan and 3.8 g. EtCOCl in PhNO₂ and on the following day gave 79% 6-methoxy-7-propionyl-1,4-benzodioxan (I), m. 81-2°, which heated with HONH₂.HCl in 50% AcOH 25 min. gave 6-methoxy-7-propionamido-1,4-benzodioxan, m. 75.5-6.5°, also formed from 6-methoxy-7-amino-1,4-benzodioxan and (EtCO)₂O. Reduction of I with LiAlH₄ gave 6-methoxy-7-(1-hydroxypropyl)-1,4-benzodioxan, b₂ 163-5°. I heated with granulated Zn and HgCl₂ solution in aqueous alc. HCl 4 hrs. gave 6-methoxy-7-propyl-1,4-benzodioxan,

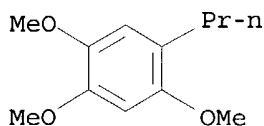
b2

131-2°, 1.5340. Elementary mol. orbital calcns. made for electron ds. in 3,4-dimethylphenol, 6-hydroxy-1,4-benzodioxan and its 5-hydroxy isomer showed differences that accounted for the differences in their chemical behavior above. The N.M.R. signals of the Me groups in 4-methylveratrole, 6-methyl-1,4-benzodioxan, its 5-Me analog, 4,5-dimethylveratrole, 6,7-dimethyl-1,4-benzodioxan, and 5,6-dimethyl-1,3-benzodioxole were reported. The last substance showed a considerable difference in spin-spin interaction of Me group protons with the various ring protons, which indicated greater degree of conductivity of conjugation effect through the 4,5-bonds in the molecule (Nair and Gopakumar, CA 60, 15701b).

IT 6906-65-6, Benzene, 1,2,4-trimethoxy-5-propyl-
(preparation of)

RN 6906-65-6 CAPLUS

CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



L8 ANSWER 14 OF 14 CAOLD COPYRIGHT 2004 ACS on STN

AN CA65:8851d CAOLD

TI oxa compds. - (VI)

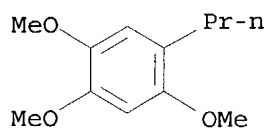
AU El'tsov, A. V.; Minkin, V. I.; Tsereteli, I. Yu.

IT 6906-65-6

RN 6906-65-6 CAOLD

CN Benzene, 1,2,4-trimethoxy-5-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

09/652,376



=> d 14 all

L8 ANSWER 14 OF 14 CAOLD COPYRIGHT 2004 ACS on STN
AN CA65:8851d CAOLD
TI oxa compds. - (VI)
AU El'tsov, A. V.; Minkin, V. I.; Tsereteli, I. Yu.
IT 6906-64-5 6906-65-6 6906-66-7 6906-67-8 6906-68-9
6906-69-0 6906-70-3 6916-51-4 6916-52-5

=> calamus oil and hydrogenat?

CALAMUS IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> s calamus oil and hydrogenat?

L9 7 CALAMUS OIL AND HYDROGENAT?

=> dup rem l9

DUPLICATE IS NOT AVAILABLE IN 'CAOLD'.

ANSWERS FROM THESE FILES WILL BE CONSIDERED UNIQUE
PROCESSING COMPLETED FOR L9

L10 7 DUP REM L9 (0 DUPLICATES REMOVED)

=> d 1-7 bib ab

L10 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:777737 CAPLUS
DN 139:292100
TI Formation of neolignan by DDQ mediated dimerization of dihydroasarone
IN Sinha, Arun Kumar; Joshi, Bhupendra Prasad; Acharya, Ruchi
PA Council of Scientific and Industrial Research, India
SO PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003080551	A1	20031002	WO 2002-IN73	20020327
	W:				
	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				
	CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,				
	GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,				
	LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,				
	PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,				
	UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,				
	TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,				
	CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,				
	BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRAI	WO 2002-IN73		20020327		
OS	CASREACT 139:292100				

09/652,376

AB The present invention relates to a novel neolignan 3-ethyl-2-methyl-3-(2'',4'',5''-trimethoxyphenyl)-1-(2',4',5'-trimethoxyphenyl)-1-propene and a process for the preparation of high purity, high yield neolignan, α -asarone, and 2,4,5-trimethoxyphenylpropionone from β -asarone or β -asarone rich Acorus calamus oil containing α - and γ -asarone by hydrogenating and dimerizing by treatment with DDQ in presence of an organic acid.

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2003:777446 CAPLUS

DN 139:292099

TI DDQ-mediated one step dimerization of β -asarone or β -asarone rich Acorus calamus oil in the formation of novel neolignan

IN Sinha, Arun Kumar; Joshi, Bhupendra Prasad; Acharya, Ruchi

PA Council of Scientific & Industrial Research, India

SO U.S. Pat. Appl. Publ., 20 pp.

CODEN: USXXCO

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2003187306	A1	20031002	US 2002-108269	20020328
	US 2004049085	A1	20040311	US 2003-660556	20030912
PRAI	US 2002-108269	B3	20020328		

OS CASREACT 139:292099

AB The present invention relates to a novel neolignan, 3-ethyl-2-methyl-3-(2'',4'',5''-trimethoxyphenyl)-1-(2',4',5'-trimethoxyphenyl)-1-(2',4',5'-trimethoxy)phenyl-1-propene [NEOLASA-I (I)], and a process for the preparation of high purity, higher yield neolignan, α -asarone, 2,4,5-trimethoxy-phenylpropionone from β -asarone (II) or β -asarone rich Acorus calamus oil containing α - and γ -asarone by hydrogenating and dimerizing by treatment with DDQ in presence of an organic acid.

L10 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2003:524051 CAPLUS

DN 139:90404

TI Process for the preparation of pharmacologically active α -asarone from toxic β -asarone-rich Acorus calamus oil

IN Sinha, Arun Kumar; Joshi, Bhupendra Prasad; Acharya, Ruchi

PA Council of Scientific & Industrial Research, India

SO U.S., 22 pp.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6590127	B1	20030708	US 2002-107844	20020328
	WO 2003082786	A1	20031009	WO 2002-IN94	20020328
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,				

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CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2002-107844 A 20020328

AB The present invention relates to a process for the preparation of high purity and yield α -asarone, trans-2,4,5-trimethoxycinnamaldehyde, and 2,4,5-trimethoxyphenylpropanone, from β -asarone or β -asarone-rich Acorus calamus oil containing α and γ -asarone by hydrogenation, followed by treatment with a dehydrogenating agent dichlorodicyanobenzoquinone (DDQ) with or without solid support of silica gel or alumina in dry organic solvent. α -Asarone can also be obtained by treating the hydrogenated product of β -asarone or β -asarone-rich A. calamus oil with DDQ in an aqueous organic solvent to obtain an intermediate 2,4,5-trimethoxyphenylpropanone, which in turn is reduced with sodium borohydride to obtain the corresponding 2,4,5-trimethoxyphenylpropanol and followed by final treatment with a dehydrating agent.

RE.CNT 91 THERE ARE 91 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:221245 CAPLUS

DN 136:247399

TI Process for the preparation of 1-propyl-2,4,5-trimethoxybenzene from toxic β -asarone of Acorus calamus or from crude calamus oil containing β -asarone

IN Sinha, Arun Kumar

PA Council of Scientific and Industrial Research, India

SO U.S. Pat. Appl. Publ., 16 pp., Division of U.S. Ser. No. 652,376.

CODEN: USXXCO

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
PI	US 2002035299	A1	20020321	US 2001-957867	20010921
	US 6528041	B2	20030304		
	CN 1340494	A	20020320	CN 2001-119219	20010327
	JP 2002088004	A2	20020327	JP 2001-101894	20010330
	US 2003113275	A1	20030619	US 2003-338327	20030108
PRAI	US 2000-652376	A3	20000831		
	US 2001-957867	A3	20010921		

OS CASREACT 136:247399

AB The invention relates to a process for the preparation of 1-Propyl-2,4,5-trimethoxybenzene useful as a aroma mol. and as a starting material and intermediate for preparation of various drugs. The process comprises providing crude calamus oil or β -asarone in a solvent; hydrogenating the solution in the presence of a catalyst; filtering the catalyst and removing the solvent under reduced pressure; subjecting the reduced calamus oil to column of silica gel chromatog. using an eluent to obtain the desired product in liquid form with 85-97% purity.

L10 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1987:72677 CAPLUS

DN 106:72677

TI Isolation and synthesis of (Z,Z)-4,7-decadienal, the character impact compound in the oil of Acorus calamus L

AU Van Lier, F. P.; Van der Linde, L. M.; Van der Weerd, A. J. A.

CS Org. Res. Dep., Naarden Int., Bussum, 1400 CA, Neth.

SO Prog. Essent. Oil Res., Proc. Int. Symp. Essent. Oils, 16th (1986), Meeting Date 1985, 215-25. Editor(s): Brunke, Ernst-Joachim. Publisher: de Gruyter, Berlin, Fed. Rep. Ger.

CODEN: 55BIAR

DT Conference

LA English

AB A number of aldehydes, many not previously found, were isolated from A. calamus oil. The syntheses of (Z,Z)-4,7-decadienol (I) [104188-11-6], (Z)-4- [68820-32-6] and (Z)-5-undecenal [68464-53-9], (Z,Z)-4,7-undecadienol [104188-12-7], and (E)-2-butyl-2-octenal [64935-38-2] were carried out for proof of structure and to correlated odors of the oils with the compds. Thus, I was prepared by ozonolysis of (Z,Z)-1,5-cyclooctadiene followed by oxidation with FeCl₃ of the methoxy hydroperoxide to give (Z)-ClCH₂CH₂CH:CHCH₃CH₂CH(OMe), iodine exchange, treatment with Ph₃P and Wittig reaction of (Z)-Ph₃P+CH₂CH₂CH:CHCH₂CH₂CH(OMe)₂ with the appropriate aldehydes. A number of other aldehydes were prepared with this Wittig compound. The odor of I most closely resembled that of A. calamus oil.

L10 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1955:86792 CAPLUS

DN 49:86792

OREF 49:16355h-i,16356a-c

TI Advancements in the chemistry of sesquiterpenes

AU Sorm, Frantisek

SO Magyar Tudomanyos Akad. Kemiai Tudomanyok Osztalyanak Kozlemenyei (1953), 3, 351-66

DT Journal

LA Unavailable

AB cf. C.A. 47, 9944c. Sesquiterpene hydrocarbons were isolated and identified by distillation combined with chromatographic adsorption on alkaline Al₂O₃ and infrared spectrophotometry. It is possible to sep. sesquiterpenes differing in number of double bonds or in C skeletons. The infrared spectra of caryophyllene from clove oil, oil of wormwood, and oil of bergamot were compared with the spectra of γ -cadinene and δ -cadinene from oil of citronella ϵ -cadinene from ylang-ylang oil, cadinene regenerated from l-cadinene-HCl, tetrahydro- γ -cadinene, tetrahydro- δ -cadinene, and cadinane from regenerated cadinene. The explanation of structures of unknown compds. was aided by hydrogenation and elimination of functional groups of the sesquiterpenes in order to compare the skeleton with known saturated hydrocarbons. By this method the structures of 2 diterpene hydrocarbons, C₂₀H₃₀ and C₂₀H₃₂, isolated from oil of wormwood were clarified. The infrared spectra of the partially hydrogenated aromatic diterpene, C₂₀H₃₀, were shown to be similar to that of 2,6-dimethyl-10-(p-tolyl)undecane. The structures of monocyclic sesquiterpenes of the bisabolane, humulene, and elemol (I) type were discussed. The skeleton of I appears to be 1-methyl-1-ethyl-2,4-diisopropylcyclohexane. Dicyclic sesquiterpenes such as cadinene, calacorene, caryophyllene, caratol, chamazulene, and the isomeric acorone and isoacorone (from calamus oil) were discussed and structures suggested for them.

L10 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

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TI Advancements in the chemistry of sesquiterpenes

AU Sorm, Frantisek

CS Stockholm

SO XIIIth Intern. Congr. Pure Appl. Chem. (1953), (Collection Czechoslov. Chem. Commun. Suppl. 2), 19,68-80

DT Journal

LA German

AB cf. C.A. 47, 9944c. Sesquiterpene hydrocarbons were isolated and

09/652,376

identified by distillation combined with chromatographic adsorption on alkaline Al₂O₃ and infrared spectrophotometry. It is possible to sep. sesquiterpenes differing in number of double bonds or in C skeletons. The infrared spectra of caryophyllene from clove oil, oil of wormwood, and oil of bergamot were compared with the spectra of γ -cadinene and δ -cadinene from oil of citronella ϵ -cadinene from ylang-ylang oil, cadinene regenerated from 1-cadinene-HCl, tetrahydro- γ -cadinene, tetrahydro- δ -cadinene, and cadinane from regenerated cadinene. The explanation of structures of unknown compds. was aided by hydrogenation and elimination of functional groups of the sesquiterpenes in order to compare the skeleton with known saturated hydrocarbons. By this method the structures of 2 diterpene hydrocarbons, C₂₀H₃₀ and C₂₀H₃₂, isolated from oil of wormwood were clarified. The infrared spectra of the partially hydrogenated aromatic diterpene, C₂₀H₃₀, were shown to be similar to that of 2,6-dimethyl-10-(p-tolyl)undecane. The structures of monocyclic sesquiterpenes of the bisabolane, humulene, and elemol (I) type were discussed. The skeleton of I appears to be 1-methyl-1-ethyl-2,4-diisopropylcyclohexane. Dicyclic sesquiterpenes such as cadinene, calacorene, caryophyllene, caratol, chamazulene, and the isomeric acorone and isoacorone (from calamus oil) were discussed and structures suggested for them.

=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

110.54

423.36

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-14.70

-14.70

STN INTERNATIONAL LOGOFF AT 18:02:22 ON 19 AUG 2004